

Scientific Computing: Cosmic Frontier Theory

HEP staff:

Salman Habib, Katrin Heitmann HEP post-docs:

Sanghamitra Deb, Juliana Kwan*, Adrian Pope, Amol Upadhye

Argonne Leadership Computing Facility (ALCF) staff:

Tim Williams

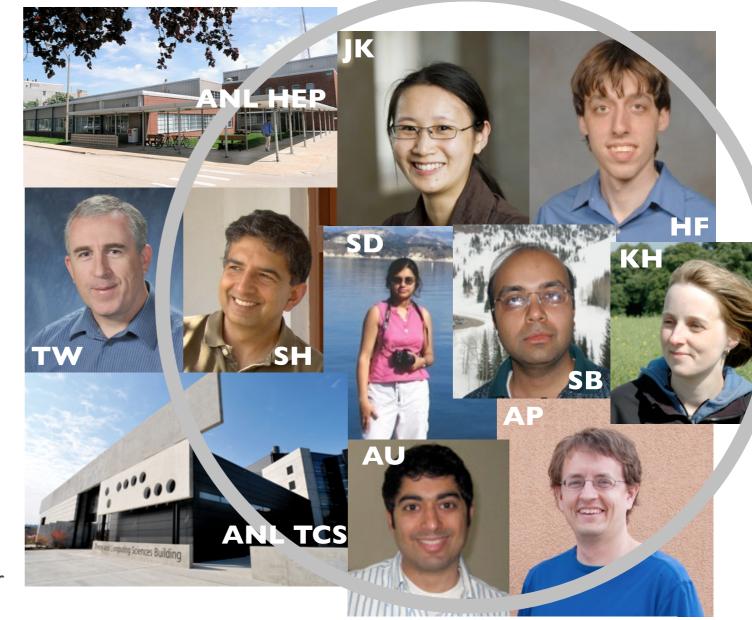
ALCF post-doc:

Hal Finkel

HEP/UChicago CMB post-doc:

Suman Bhattacharya

*joining October







Precision Cosmology: Modeling and Observations

Early Period (1980's)

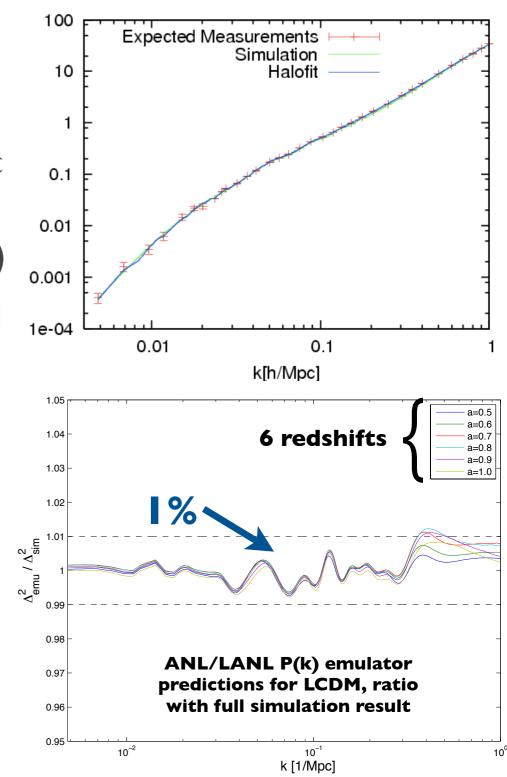
- Access to large data choked (technology did not exist), insignificant computing
- Characterized by small datasets, 'eyeball' comparisons, simple statistics

Intermediate Phenomenology (current, ~10%)

 Use simulation to build intermediate, simplified theoretical model; use this to interact with observations (HOD models, HaloFit, scaling relations from simulations, --)

'Direct' Numerics (future, ~1%)

 'Theory' = direct interaction with observations by sophisticated simulations (or intermediate numerical products, 'emulators'); complex space -- understand systematic errors (missing/wrong physics), bias





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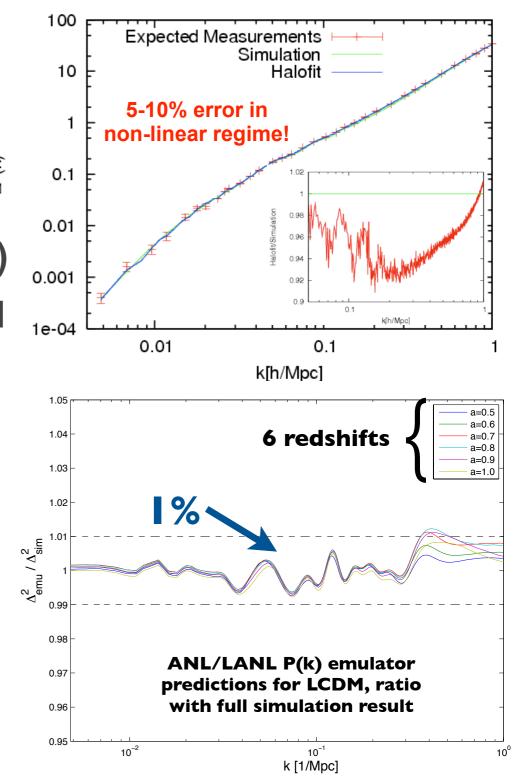
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Effort Base: The HACC Framework

Basic Requirements

- Large (~trillion particle) N-body simulations covering a wide parametric range with controlled accuracy
- Sophisticated analysis framework (on the fly and post-processing)
- Run 'at scale' simulations to build emulators and explore parameters
- Ability to run across multiple supercomputer architectures
- Hardware/Hybrid Accelerated Cosmology Code (HACC) Framework Status
 - Production on CPU/Cell systems
 - Version for CPU/GPU ready for 'at scale' tests
 - Port to Blue Gene architectures nearing completion (also ports HACC to multi-core CPU systems), excellent work by Nick Frontiere (UG)
 - Starting to look at Intel's MIC architecture
 - Continue work on development of analysis suite (primarily at CPU level)
 - Multiple invited talks (Titan summit, Germany, ICiS, Oklahoma, --)



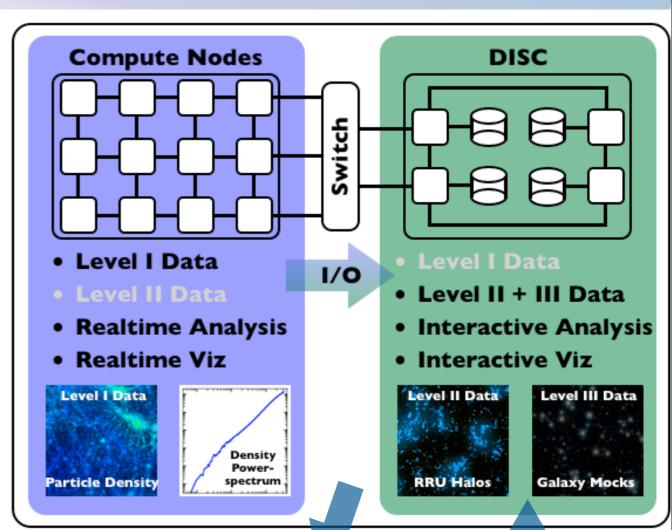
'Ultimate Vision'

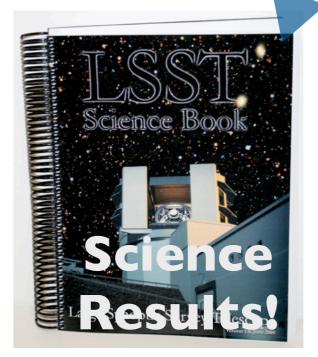
- 'Discovery Space': Robust theory with subtle signals
- Precision Cosmic Calibration at Scale: 'All Sky' solution of the cosmic inverse problems in the nonlinear regime
- Cosmology Simulations at the Exascale: Next-generation computing and beyond as essential theoretical and analysis tool -- genesis of HACC





- Large Data: Simulation & observational datastreams: Archiving, serving, quality assurance, (joint) analyses
- Simulation/Data/Analysis: Crossplatform, multi-source, analysis and interrogation frameworks









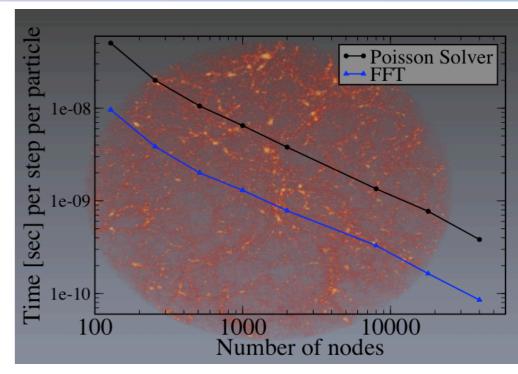
Building Collaborations: ANL ALCF/CI/MCS

Argonne Leadership Computing Facility

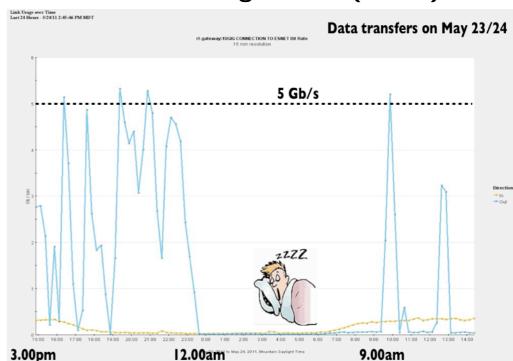
- Mira 10 PFs IBM BG/Q "Dark Universe" ESP project
- Working with Catalyst (R. Balakrishnan, T. Williams), Data Analytics & Visualization & Storage Resources (M. Hereld), Performance Engineering (K. Kumaran, V. Morozov) teams

Computation Institute (ANL/UChicago)

- Data serving (I. Foster, T. Malik) and high bandwidth data transfer (R. Kettimuthu)
- Mathematics & Computer Science Division
 - Space in TCS building for staff and post-docs
 - Working with Distributed Systems Laboratory (R. Ananthakrishnan) and Futures Laboratory (J. Insley, M. Papka, T. Peterka), I/O (R. Ross, V. Vishwanath), parallel libraries (R. Thakur)



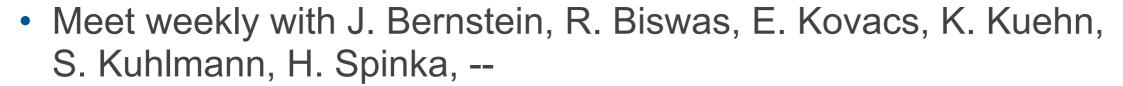
Scaling of HACC solvers on the full BG/P (above), high-rate data transfers from LANL to ANL using Globus (below)

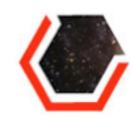




Building Collaborations: ANL HEP Division

Interactions with DES team





- Membership in DES collaboration proposed for S. Bhattacharya, S. Deb,
 S. Habib, K. Heitmann, J. Kwan, and A. Pope (HACC simulations, emulation of weak lensing observables, galaxy clustering, clusters)
- Interactions with SPT CMB effort: Joint Post-Doc
 - Post-doc S. Bhattacharya with J. Carlstrom (SZ clusters, CMB lensing)
- Theory for Direct/Indirect Dark Matter search experiments
 - With HE astrophysicists (K. Byrum, G. Decerprit, R. Wagner, B. Zitzer, et al.)
- 'Large Data' Opportunity with HEP Experimentalists
 - Significant synergy with interests in D. Malon's group (e.g., LSST, data serving help from Q. Zhang); ICiS workshop in August 2011
- Theory Group
 - Exploring several interests (dark energy/matter, quantum gravity effects, --)



Chicagoland Collaborations

Fermilab

- Discussing weak lensing collaboration with S. Dodelson and collaborators, DES work with J. Frieman
- Possible collaborations with N. Gnedin on several baryonic simulation problems
- Significant computing and large data interests being explored with E. Gottschalk and J. Kowalkowski

University of Chicago

 S. Habib and K. Heitmann (on KICP postdoc committee) are Senior Members of the Kavli Institute for Cosmological Physics (KICP); computational collaborations possible with A. Kravtsov

Computation Institute

- Several interests with FLASH Center (D. Lamb)
- New ideas in particle simulation methods with F. Catteneo and R. Rosner
- CI connections being explored



National Lab HEP Computational Cosmology Collaboration



- ANL, BNL, FNAL, LBNL, SLAC (plus university partners)
 - Much work has gone in towards building a computational cosmology collaboration centered around the HEP Labs: presentation post-HEPAP in Washington DC, June 24; Aug 18/19 workshop at LBNL; planning meeting Sep 13/14 in Washington DC (with ASCR, HEP, & NSF program management present)
 - Near-term concrete work steps have been outlined, a meeting report from the September Washington DC meeting will be available in earlymid October
 - Major NERSC request submitted (first large collaboration proposal for cosmology); HEP SciDAC call has explicitly asked for cosmology as one of three focus areas
 - Provides new opportunities for work with HEP computation in the experimental programs, with accelerator physicists, and for connections to ASCR, and, as appropriate, to NASA and NSF



Computational Cosmology and HPC: Connections to ASCR

Parallel Simulations

 Early parallelization of all codes, efficient utilization of supercomputing resources (several Gordon Bell prizes, including use of custom hardware)

More Physics: Multi-Physics/Multi-Resolution

 Several current cosmology codes have complexity similar to combustion codes, others are aimed at optimizing performance and memory (survey scale simulations); all add to ASCR capabilities suite

Next-Generation Architectures

 Increased concurrency with communication bottlenecks and costs -- codes must evolve to deal with these problems; major issue for ASCR







'Large Data': The Connection with HEP Experiments

Digital Data

 CCD sky surveys, SDSS (10s of TB), many 'use' modes -- very rich scientifically

Next-Generation Surveys

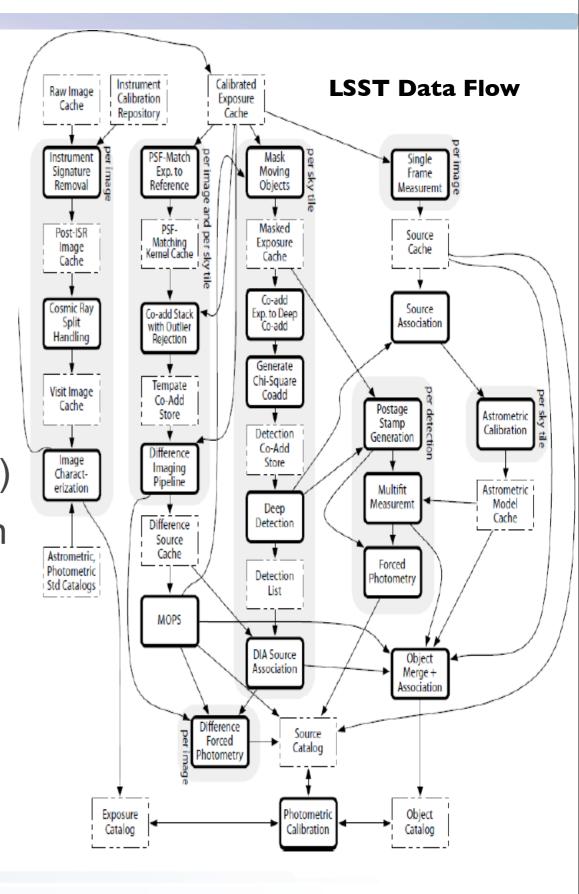
DES starting (~PB); LSST coming (~100 PB)

Analysis modes

- Many 'single' applications (each complex)
- Very many cross-correlations to constrain systematics, tease out new signals

Problems of Scale

- Simulation/observational data sizes drive needs for new algorithms
- Complex workflows, high-throughput computing, large number of users





Workshops, Past and Future

- SF11 (July 4-22)
 - Santa Fe Cosmology Summer Workshops running from 1999 onwards (1/3 faculty, 1/3 post-docs, 1/3 graduate students)
- ICiS Workshop (August 6-13): Large Datasets in Astrophysics & Cosmology
 - 30 participants across domain science, computer science, HEP experiments
- Computing at the Cosmic Frontier (September 13-14)
 - Planning meeting for computational cosmology collaboration
- Future
 - 'Pow-wow' workshop with HEP experimentalists/computational scientists
 - Possible ANL 'Large Data' initiative
 - Ideas for SF12 and next ICiS workshop --

